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Surface Science Letters

Influence of a spin-polarized tip on the Fe(001) surface

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Abstract

A detailed study of ab initio calculations for an iron parallel electrode and a tip–surface system, using the localized spherical wave method and the supercell-slab approach is presented. The calculations show that within the medium inter-electrode distance range (about 2.9 to 5.7 Å) the interaction between two parallel electrodes has a strong influence on the local surface electronic structure, while the magnetic moment is almost constant. A tip induces changes of the specific surface states near the Fermi level. However, the spin-polarization of the tip shows no significant influence on the surface states. © 1999 Elsevier Science B.V. All rights reserved.

Keywords: Density functional calculations; Iron (001) surface states; Spin-polarized tip

The invention of scanning-tunneling microscopy (STM) made it feasible to explore in real space the atomic-scale realm of solid surfaces [1–4]. A theoretical treatment of the STM was first presented by Tersoff and Hamann (TH), who concluded that the tunneling current is proportional to the local density of states of the surface, at the position of the tip [5]. Subsequently, Lang [6,7] confirmed the conclusion by the computation of the tunneling-current density in the vacuum region between two planar metal electrodes, with on each of them an adsorbed atom. Experimentally, Stroscio et al. found sharp specific features near the Fermi energy in the scanning-tunneling spectroscopy (STS) of the bcc (001) surface of Fe

and Cr [8]. Such element-specific features have been used to study the growth and alloying of Cr on the Fe(001) surface [9].

Recently, some authors have investigated the possibilities of applying STM, as well as other scanning probe microscopies, to reveal surface magnetic properties with a high lateral resolution. This technique is referred to as spin-polarized scanning tunneling microscopy (SPSTM) [10,11]. The use of a magnetic tip ferromagnetically or antiferromagnetically aligned with respect to the surface as the source of spin-polarized electrons in SPSTM is supported by theories [12–14] and by experiments [15]. Therefore, it is worth knowing the influence of a spin-polarized tip on the surface states.

The interaction between the sample and the tip has been the subject of several investigations [1–

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4,16–20]. Tsukada et al., using theoretical simulations from first-principles, found that the tunneling current concentrates on the single apex atom of the tip [18]. For a tip–surface distance of about 4 Å, strong tip–sample interactions exist, which may induce changes in electronic structure accompanied by significant charge rearrangements [3,16–20]. Bode et al. found experimentally different tunneling curves for a submonolayer of iron on the W(110) surface depending on the use of a tungsten tip or an iron-covered tip [21]. However, until now no *ab initio* calculations concerning the interaction between a surface and a spin-polarized tip have been reported.

Here we report the results of *ab initio* calculations for the iron (001) surface under the influence of a spin-polarized tip. Similar to previous work [6,7,18], we take a configuration where the STM-current flows between two parallel electrodes or between the surface and an adatom absorbed on parallel electrodes. A tip–surface system is composed of two separate parts: an iron tip and an iron (001) surface. An iron tip is simulated by an iron adatom on the Fe(001) surface in a supercell $a=b=2 \times a_0$ (Fig. 1b). A series of parallel electrode systems (Fig. 1a) is composed of 11 ML of iron along the (001) direction with inter-electrode distances from 2.2 to 14.8 Å. In line with earlier work [16–21] and in accord with the calculated results of the parallel electrodes, a tip–surface distance of 3.5 Å was chosen. Both spin-polariza-

tion directions for the tip were investigated. A system with a larger surface–tip distance (5.74 Å), as well as a surface without tip, was calculated for comparison. In all the calculations no structure relaxation was taken into account, because the relaxation is very small (less than 1% in distance) for the iron (001) surface system [22].

Ab initio calculations were performed with the localized spherical wave (LSW) method [23] using a scalar-relativistic Hamiltonian. We used local-spin-density exchange-correlation potentials [24] inside space-filling and, therefore, overlapping spheres around the atomic constituents. The self-consistent calculations were carried out including all core electrons. Since the magnetic properties are sensitive to the Brillouin zone sampling, a dense mesh of one k -point per 10^{-6} Å³ was employed. The Wigner–Seitz radius of iron atoms is the same as the bulk value.

Fig. 2 shows the relationship between the magnetic moment of the surface iron and the distance between two parallel electrodes. The behavior of the magnetic moment of the surface iron as a function of the inter-electrode distances shows three ranges. The surface magnetic moment strongly increases with increasing the inter-electrode distance when the distance is short (<2.88 Å). This is due to the strong overlap between the surface irons, especially between the

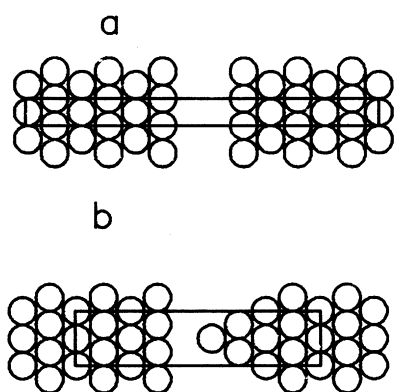


Fig. 1. Schematic representation of the iron (001) parallel electrode system (a) and the iron tip–surface system (b). The boxed regions indicate the unit cells.

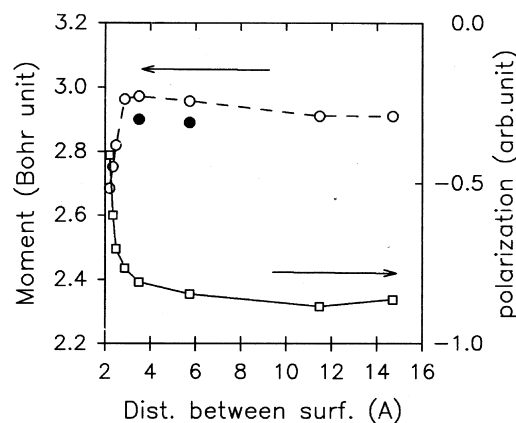


Fig. 2. The relationships between the magnetic moment (circles) and spin polarization (squares) of the iron(001) surface and the inter-electrode distance for the parallel electrode system. The filled circles represent the magnetic moment of the Fe(001) under a tip.

3d states. The surface Fe magnetic moment reaches the maximum at about $2.96 \mu_B$ when the inter-electrode distance is increased to 2.88 \AA (about the length of the a -axis of the bcc Fe). In the distance range from about 2.88 to 5.74 \AA , the magnetic moment remains almost constant, while the number of electrons increases (from 7.45 electrons for $d=2.88 \text{ \AA}$ to 7.50 electrons for $d=5.74 \text{ \AA}$). These results indicate that in the medium distance range the interaction between the two electrodes is not due to the iron 3d–3d states. The calculations also show that the magnetic moment of the surface Fe converges to $2.91 \mu_B$ when the inter-electrode distance is larger than about 6 \AA . The electrode does not have an influence on the Fe (001) surface states when the inter-electrode distance is reasonably large ($>6 \text{ \AA}$).

The densities of states of the surface irons with an inter-electrode distances ranging up from 2.88 \AA are shown in Fig. 3. The 3d band the surface iron for the majority electrons is almost fully occupied. The influence of a parallel electrode on the surface iron is mainly on the 3d band of the minority electrons: with increasing inter-electrode distance, the unoccupied 3d band become narrower; the density of the 3d states at energies $\sim -0.1 \text{ eV}$ and about 1.1 eV increases, as shown in Fig. 3. The

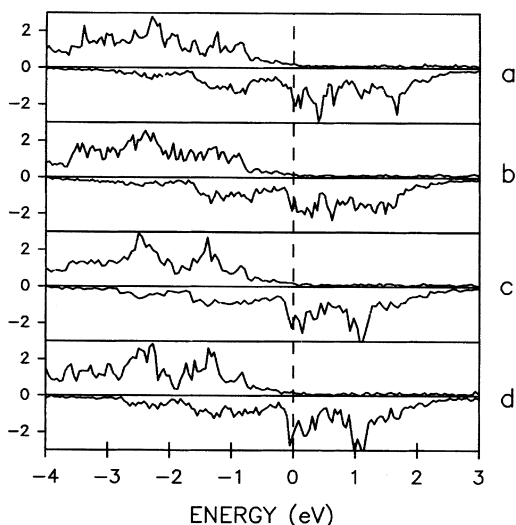


Fig. 3. Local density of states for the Fe(001) in the electrode systems with the inter-electrode distance: (a) 2.88 \AA , (b) 3.50 \AA , (c) 5.74 \AA , and (d) 14.80 \AA . The Fermi level is at 0 eV .

density of the 3d state $\sim -0.1 \text{ eV}$ is regarded as a specific feature for the bcc iron (001) surface, which is strongly influenced by the existence of the other parallel electrode. Experiments showed this specific feature at about 0.17 eV above the Fermi level [8], which we will discuss later in the paper.

Fig. 2 also includes the spin-polarization of the surface iron at the Fermi energy, which is defined as $p = (n_+ - n_-)/(n_+ + n_-)$; here n_+ represents the density of states at the Fermi level for the majority electrons, and n_- that of the minority electrons. The spin-polarization for the surface iron is all negative and reversed to the bulk value (about $+35\%$) [25]. It changes strongly with the inter-electrode distance when the distance is shorter than 2.88 \AA , and become almost constant from the medium distance (3.5 \AA).

Now we discuss the iron (001) surface under the spin-polarized tip with the tip–surface distance of 3.5 \AA . The magnetic moment of the surface iron in the presence of a tip is about $2.89 \mu_B$, slightly reduced compared with the clean iron (001) surface ($2.91 \mu_B$), which is in contrast to the enhancement by a parallel electrode, as shown in Fig. 2. The local density of states is very similar to that of the clean surface. However, there are some differences, of which the most significant one is the position of the specific features around the Fermi level: the position of the surface states, about -0.1 eV for the clean Fe(001) surface (Fig. 3d), has shifted to about 0.1 eV above the Fermi level under the influence of a spin-polarized tip (Fig. 4). There is a small shoulder in the energy about -0.1 eV in the local density of states. This small but significant shift explains the difference between the calculated (about -0.1 eV) and the experimental data (about 0.17 eV above the Fermi level [8,9]) for the iron surface states. Fig. 4 also includes the local density of states for the iron (001) surface under the tip with a tip–surface distance of 5.74 \AA , there are two peaks at about -0.1 eV and about 0.1 eV .

The spin-polarization of the tip has almost no influence on the local density of states of the surface, as shown in Fig. 4. This is due to the fact that the interactions between the tip and the surface are mainly between the iron 4s, 4p states, as well as between the iron 4s, 4p on one side of the

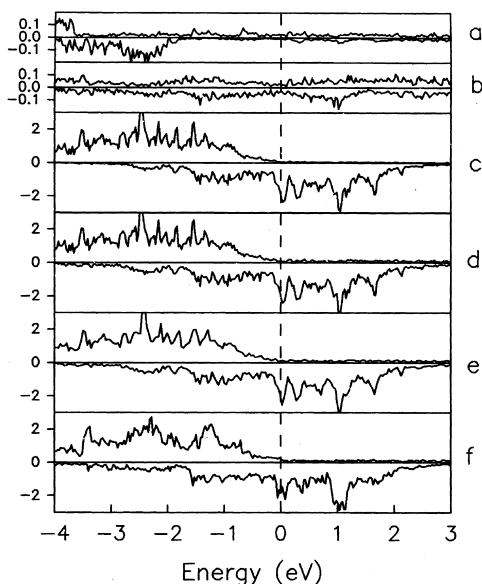


Fig. 4. Local density of states for the Fe(001) in the presence of a tip: (a)–(d): tip–surface distance of 3.5 Å, magnetization of tip and surface parallel: (a) Fe 4s, (b) Fe 4p, (c) Fe 3d and (d) total density of states; (e) as (d) but magnetization of tip and surface anti-parallel; (f) total density of states for the Fe(001) with tip and surface magnetization parallel and a tip–surface distance of 5.74 Å. The Fermi level is at 0 eV.

system and the 3d states on the other side, and vice versa, but not through direct 3d–3d interactions. The iron 4s and 4p states of the tip and the surface show little spin-polarization, as shown in Figs. 4 and 5.

Here we give a brief discussion of our calculated results in relation to the experimental data for the Fe(001) surface. Stroscio and coworkers found that there is a specific feature of the surface states at an energy of about 0.17 eV [8,9]. In another STM(S) experiment Biedermann et al. found that the peak of the Fe(001) surface states is at the energy about 0.3 eV above the Fermi level [26]. They also found that the position of the surface states may change in the energy range from 0.2 to 0.3 eV, depending on the tips [27]. Our calculations show that the clean Fe(001) surface has a peak at about 0.1 eV below the Fermi level. The application of an iron tip shifts the position of the surface states from -0.1 eV to about 0.1 eV above the Fermi level. This shifted position of the Fe(001)

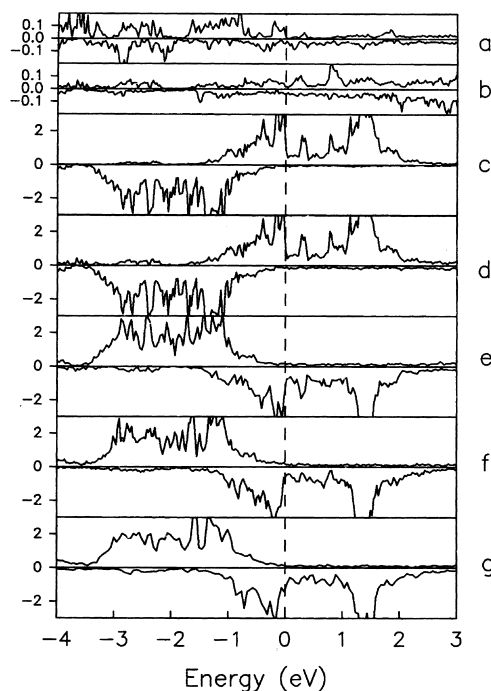


Fig. 5. Local density of states for the Fe tip in the tip–surface systems: (a)–(d) belongs to a ferromagnetic tip with a tip–surface distance of 3.5 Å: (a) Fe 4s, (b) Fe 4p, (c) Fe 3d and (d) total density of states; (e) total density of states for an antiferromagnetic tip with a tip–surface distance of 3.5 Å; (f) total density of states for a ferromagnetic tip with a tip–surface distance of 5.74 Å; (g) total density of states for an iron tip. The Fermi level is at 0 eV.

surface states is in better agreement with the experiments.

In conclusion, we performed ab initio calculations for iron surface–tip systems. The calculations show interactions between the tip and the surface. Such interactions induce the change of the position of the iron specific states from -0.1 eV to 0.1 eV above the Fermi level. The calculated results explain the difference between the band structure calculations and experimental data, as well as confirm the sensitivity of the surface states on the tip geometry.

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References

- [1] G. Binnig, H. Rohrer, *Helv. Phys. Acta* 55 (1982) 726.
- [2] G. Binnig, H. Rohrer, C. Gerber, E. Weibel, *Phys. Rev. Lett.* 50 (1983) 120.
- [3] F. Besenbacher, *Rep. Prog. Phys.* 59 (1996) 1737.
- [4] L.E.C. van de Leemput, H. van Kempen, *Rep. Prog. Phys.* 55 (1992) 1165.
- [5] J. Tersof, D.R. Hamann, *Phys. Rev. B* 31 (1985) 805.
- [6] N.D. Lang, *Phys. Rev. Lett.* 55 (1985) 230.
- [7] N.D. Lang, *Phys. Rev. B* 34 (1986) 5947.
- [8] J.A. Stroscio, D.T. Pierce, A. Davies, R.J. Celotta, M. Weinert, *Phys. Rev. Lett.* 75 (1995) 2960.
- [9] A. Davies, J.A. Stroscio, D.T. Pierce, R.J. Celotta, *Phys. Rev. Lett.* 76 (1996) 4175.
- [10] M.W.J. Prins, H. van Kempen, H. van Leuken, R.A. de Groot, W. van Roy, J. De Boeck, *J. Phys.: Condens. Matter* 7 (1995) 9447.
- [11] R. Laiho, H.J. Reittu, *J. Phys.: Condens. Matter* 9 (1997) 5697.
- [12] A.A. Minoakov, I.V. Shvets, *Surf. Sci.* 236 (1990) L377.
- [13] J.C. Slonczewski, *Phys. Rev. B* 39 (1989) 6995.
- [14] E.Yu. Tsymbal, D.G. Pettifor, *J. Phys. Condens. Matter* 9 (1997) L411.
- [15] R. Wiesendanger, H.-J. Guntherodt, G. Guntherodt, R.J. Gambino, R. Ruf, *Phys. Rev. Lett.* 65 (1990) 247.
- [16] S. Ciraci, A. Baratoff, I.P. Batra, *Phys. Rev. B* 41 (1990) 2763.
- [17] G. Doyen, D. Drabova, J.V. Barth, R. Schuster, T. Gritsch, R.J. Behm, G. Ertl, *Phys. Rev. B* 48 (1993) 1738.
- [18] M. Tsukada, K. Kobayashi, N. Isshiki, H. Kageshima, *Surf. Sci. Rep.* 13 (1991) 265.
- [19] A.L. Vazquez de Parga, O.S. Herman, R. Miranda, A. Levy Yeyati, N. Mingo, A. Martin-Rodero, F. Flores, *Phys. Rev. Lett.* 80 (1998) 357.
- [20] Y. Kuk, P.J. Silverman, *J. Vac. Sci. Technol. A*: 8 (1990) 289.
- [21] M. Bode, R. Pascal, R. Wiesendanger, *J. Vac. Sci. Technol. A*: 15 (1997) 1285.
- [22] S. Handschuh, S. Blugel, *Solid State Commun.* 105 (1998) 633.
- [23] H. van Leuken, A. Lodder, M.T. Czyzyk, F. Springelkamp, R.A. de Groot, *Phys. Rev. B* 41 (1990) 5613.
- [24] L. Hedin, B.I. Lundqvist, *J. Phys. C* 4 (1971) 2064.
- [25] C.M. Fang, R.A. de Groot, M.M.J. Bishop, H. van Kempen, *Phys. Rev. B* 58 (1998) 6773.
- [26] A. Biedermann, O. Genser, W. Heberstreit, M. Schmid, J. Redinger, R. Podloucky, P. Varga, *Phys. Rev. Lett.* 76 (1996) 4179.
- [27] M. Schmid, personal communication.